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Factor screening by sequential bifurcation

Bettonvil, B.W.M.

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5000 LE TILBURG
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FACTOR SCREENING BY SEQUENTIAL
BIFURCATION

Bert Bettonvil

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FACTOR SCREENING BY SEQUENTIAL BIFURCATION.

Bert Bettonvil

Catholic University Tilburg/Technical University Eindhoven

P O Box 90153

5000 LE Tilburg

Netherlands

In order to screen the input variables in simulation problems without noise we propose a modification of sequential bifurcation, a method resembling the binary search technique. Our method turns out to be very efficient in comparison to other techniques.

(SIMULATION,SCREENING)

1. Introduction.

Suppose we are faced with a simulation problem in which a great many (100,1000,10000?) input variables can be varied, but we think that just a few of these are really important. To find out which of the variables are important, the one-factor-at-a-time method runs a basic simulation with all variables at one level and - in case of N variables - N extra simulation runs; in each run one variable is at another level and $N-1$ variables are at the basic level. A more effective method uses a Resolution-III design where the number of runs equals $N+1$, rounded up to the next multiple of four; see Box and Hunter (1961a,b). But a simulation run can be very time-consuming, in which case simulating N or more runs is prohibitive.

A number of techniques have been developed to tackle this problem. In this paper we propose a modification of sequential bifurcation. This technique was introduced by Jacoby and Harrison (1962) for error-free observations. Our modification makes sequential bifurcation (or "SB") even

more efficient; actually SB is very efficient compared to the other existing techniques, as the examples will show.

In this paper we restrict ourselves to observations without random error. A paper on SB in situations with random error is in preparation.

In section 2 of this paper we describe our version of SB and introduce a special notation. In section 3 we derive the maximum number of runs needed to find k important variables out of N candidate variables. In section 4 we use this number to compare our version of SB to other techniques that tackle the same problem. In section 5 conclusions are drawn and suggestions for further investigation are made.

2. Description and notation.

Suppose the simulation outcome y can be expressed as a first-order linear model of N variables $x_1, x_2, \dots, x_N$:

$$y = y(x_1, x_2, \dots, x_N) = \beta_0 + \beta_1 x_1 + \dots + \beta_N x_N. \quad (2.1)$$

A crucial assumption is, that there is a priori knowledge of the direction of the influence of each x_i ($i=1, \dots, N$), if such an influence is present at all. Consequently, we can recode x_i to achieve that all variables have positive influence. So we assume $\beta_i \geq 0$ ($i=1, \dots, N$). We do not know which of the β 's are positive, nor do we know the number of positive β 's, but we expect this number to be small.

Our version of SB is a modification of the Jacoby and Harrison (1962) approach. For sake of convenience we assume that $N=2^m$; if not, we can add dummy variables to the model (with β_i known to be zero) to achieve this. For all independent variables we may restrict ourselves to two levels, that we can denote as "low" and "high", or "off" and "on", or "0" and "1". We begin our search for the important variables by performing a simulation run with all independent variables at their low levels, and a simulation run with all x_i at their high levels. The difference in their outcomes equals the sum of all regression parameters, which are all non-negative. So if this difference

is zero, all parameters are zero, and our problem is solved using only two simulation runs. However, if the difference is positive, then one or more parameters are positive.

In that case, we next perform a simulation run with half of the variables at their low levels, the other half at their high levels (bifurcation). Without loss of generality we may take the second half of the x-variables at their high levels. One of three things will happen.

(i) The latest outcome may equal the outcome with all variables low; this means that the second half of the x_i 's does not matter, and we have to investigate only the first half of the variables.

(ii) The latest outcome may be equal to the outcome with all variables high; all parameters in the first half are zero, and we restrict our search to the second half.

(iii) The outcome may be intermediate. Then there are non-zero parameters in both halves.

The next step in the sequence is performed within the half (case i and ii) or halves (case iii) that contain non-zero regression parameters. Again in that step the relevant variables are splitted up into two groups of equal size, one group at the low, the other group at the high levels; the variables not under consideration are kept low. The new simulation outcome is compared with the preceeding outcomes. This "Sequential Bifurcation" is repeated until we reach groups of size 1, i.e. individual variables.

Example 1. Suppose we are dealing with 8 variables; β_2 and β_4 are positive, the other regression parameters are zero. Our first observations are $y_1 = y(0,0,0,0,0,0,0,0)$ and $y_2 = y(1,1,1,1,1,1,1,1)$, and $y_1 < y_2$. The next simulation run gives us $y_3 = y(0,0,0,0,1,1,1,1)$, and $y_3 = y_1$, so we know that $\beta_5 = \beta_6 = \beta_7 = \beta_8 = 0$. We go on with $y_4 = y(0,0,1,1,0,0,0,0)$, for which holds that $y_1 < y_4 < y_2$, and we conclude that the first as well as the second group of two parameters has to be investigated. So we observe $y_5 = y(0,1,0,0,0,0,0,0)$ and $y_6 = y(0,0,0,1,0,0,0,0)$ which, in combination with the former observations, show that $\beta_1 = \beta_3 = 0$, and β_2 and β_4 are positive. With the use of six observations, we found out which two out of eight parameters are important.

To avoid lengthy sequences of zeros and ones in case of many parameters (and that is our topic of research), we have to introduce a special notation. In stage j ($j=0,1,\dots,m$) of our search we divide the $N=2^m$ independent variables into 2^j groups of equal size 2^{m-j} ; only the variables in one of these groups are "on"; all other variables are "off". To indicate which group we are dealing with, we introduce the following.

DEFINITION 1. The sum of the parameters in the i^{th} group, out of 2^j equally sized groups, is denoted by $\beta_{i|j}$ ($i=1,2,\dots,2^j$; $j=0,1,\dots,m$).

DEFINITION 2. $\beta_{0|0} := 0$. (We use ":@" for "is defined as".)

DEFINITION 3. $y_{i|j} := \beta_0 + \beta_{i|j}$ for all i and j for which $\beta_{i|j}$ is defined.

Consequently, the observation with all independent variables at their high levels is denoted by $y_{1|0} = \beta_0 + \beta_{1|0}$; that is, we have $2^0=1$ group, and the "first" group is "on"; the observation with all independent variables at their low levels is $y_{0|0} = \beta_0$.

So the first two observations in SB are

$$y_{0|0} = \beta_0 \quad (2.2)$$

and

$$y_{1|0} = \beta_0 + \beta_1 + \beta_2 + \dots + \beta_N. \quad (2.3)$$

By assumption, we have $\beta_i \geq 0$ ($i=1,\dots,N$), so that it is clear that $y_{0|0} \leq y_{1|0}$. If $y_{0|0} = y_{1|0}$, we can stop, as this equality can occur only if $\beta_1 = \beta_2 = \dots = \beta_N = 0$; we conclude that no factor is important. If $y_{0|0} < y_{1|0}$, we know that at least one of the β 's is positive; we continue and split the

(single) group of variables into two groups of equal size $N/2 = 2^{m-1}$, and we observe $y_{2|1} = y(0,0,\dots,0,1,1,\dots,1)$:

$$y_{2|1} = \beta_0 + \beta_{2|1} = \beta_0 + \beta_{(N/2)+1} + \beta_{(N/2)+2} + \dots + \beta_N \quad (2.4).$$

When we proceed from stage $j-1$ to stage j of the procedure, we split the independent variables of group i (at stage $j-1$) into two groups, and from definition 1 it follows that the relation between the β 's at level $j-1$ and level j is described by

$$\beta_{i|j-1} = \beta_{2i-1|j} + \beta_{2i|j} \quad (j=1,\dots,m; i=1,\dots,2^{j-1}). \quad (2.4)$$

The corresponding relation between the observations at levels $j-1$ and j is

$$y_{i|j-1} = y_{2i-1|j} + y_{2i|j} - y_{0|0} \quad (j=1,\dots,m; i=1,\dots,2^j). \quad (2.5)$$

This relation shows that observation of $y_{2i-1|j}$ is unnecessary, once $y_{0|0}$, $y_{i|j-1}$ and $y_{2i|j}$ have been observed. Of course, we could as well observe $y_{2i-1|j}$ and not observe $y_{2i|j}$, but we choose to obtain the observation with an even index, and may do so without loss of generality.

We describe our version of SB as follows:

- (1) Observe $y_{0|0}$ and $y_{1|0}$; consider $\beta_{1|0} = y_{1|0} - y_{0|0}$.
- (2) If the $\beta_{i|j}$ under consideration equals 0, all its β -components are 0;
 - if $\beta_{i|j} > 0$ and $j=m$, we have found a $\beta_i > 0$;
 - if $\beta_{i|j} > 0$ and $j < m$, proceed to step (3).
- (3) Observe $y_{2i|j+1}$ and compute
 - $\beta_{2i|j+1} = y_{2i|j+1} - y_{0|0}$ and $\beta_{2i-1|j+1} = \beta_{i|j} - \beta_{2i|j+1}$ (see (2.4));
 - proceed to both step (4a) and step (4b).
- (4a) The new β under consideration is $\beta_{2i|j+1}$; proceed to step (2).
- (4b) The new β under consideration is $\beta_{2i-1|j+1}$; proceed to step (2).

Example 2. We can now describe example 1 in a much shorter way. Our first observations are $y_0|_0$ and $y_1|_0$, with $y_0|_0 < y_1|_0$, so $\beta_1|_0 > 0$. The next observation is $y_2|_1$, with $y_2|_1 = y_0|_0$, so $\beta_2|_1 = 0$ and $\beta_1|_1 > 0$. We go on with $y_2|_2$, and as $y_0|_0 < y_2|_2 < y_1|_0$, we conclude that $\beta_1|_2 > 0$ and $\beta_2|_2 > 0$. Finally, by observing $y_2|_3$ and $y_4|_3$, we find out that $\beta_1|_3 = \beta_3|_3 = 0$, $\beta_2|_3 > 0$ and $\beta_4|_3 > 0$.

Example 3. Jacoby and Harrison give an example with $128=2^7$ variables, in which the numbers 68, 113 and 120 are the only non-zero effects. Our BS-analysis would start by observing $y_0|_0$ and $y_1|_0$, resulting in $\beta_1|_0 > 0$. The next observation is $y_2|_1$, which gives us $\beta_2|_1 = y_2|_1 - y_0|_0 > 0$ and $\beta_1|_1 = \beta_1|_0 - \beta_2|_1 = 0$, so $\beta_1 = \dots = \beta_{32} = 0$. Figure 1 represents the whole procedure. The positive parameters are underlined.

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*           Figure 1 about here      *
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Jacoby and Harrison (1962) proposed to take two observations for every group of β 's to be split, one with the first half of the variables under consideration "on", the other with the second half "on", where we utilize eq. (2.4). Their procedure demands many more observations, actually almost twice as much: in example 3 we need 16 observations, Jacoby and Harrison need 30 observations (apart from $y_0|_0$ and $y_1|_0$ all observations are doubled).

3. Number of runs in the error-free case.

To compare SB with other techniques, we compute the number of observations, necessary to find k non-zero coefficients out of $N=2^m$ non-negative ones. We restrict ourselves to worst-case (upper-limit) computations. We use the term "stage" for j as introduced in section 2, so $y_{0|0}$ and $y_{1|0}$ are observations at stage 0, $y_{2|1}$ is an observation at stage 1, etc.

Suppose $k=0$. Trivially, we need two observations: $y_{0|0}$ and $y_{1|0}$.

Suppose $k=1$. We need the observations $y_{0|0}$ and $y_{1|0}$ and one observation at each lower stage j , $j=1, \dots, m$; so we need $m+2$ observations.

As a last example, suppose $k=2$. We need the observations $y_{0|0}$, $y_{1|0}$ and $y_{2|1}$ to start. Now the two β 's are either in the same half or in different halves. If we have bad luck, they are in different halves. In that case we need two observations at each lower stage j ($j=2, \dots, m$); so in total we need $3+2(m-1)=2m+1$ observations.

Now we consider the general case. Be $k>0$. At level 0, two observations are necessary. At stage j ($j=1, \dots, m$) the number of observations is equal to the number of non-zero (accumulated) coefficients found at stage $j-1$. This number is k at most, neither can it exceed 2^{j-1} , the total number of coefficients at stage $j-1$. We can define an integer ℓ ($0 \leq \ell \leq m$) such that $2^{\ell-1} < k \leq 2^\ell$. At stage j , $j=1, \dots, \ell$, the maximum number of observations is 2^{j-1} ; this maximum applies, if the non-zero coefficients are not clustered. At stage j , $j=\ell+1, \dots, m$, we need k observations; or less, if the non-zero coefficients are clustered at this stage. Hence, in the worst case, the number of observations is

$$2 + \sum_{j=1}^{\ell} 2^{j-1} + \sum_{j=\ell+1}^m k = 1 + 2^{\ell} + k(m-\ell). \quad (3.1)$$

For small k , the number of observations is linear in k and logarithmic in N .

Example 4. In example 3 we have $128=2^7$ variables with 3 non-zero effects. So $m=7$, $k=3$, and as a consequence $\lambda=2$. The maximum number of observations, according to (3.1), is $1+2^2+3(7-2)=20$. The actual number of observations is 16 because of clustering.

4. Comparison of SB to other screening techniques.

In this section we describe a number of alternative screening techniques, and compare them to our version of SB, theoretically as well as by means of an example. We shall discuss Random Designs, Two-Stage Group-Screening, Multi-Stage Group-Screening and the original version of Sequential Bifurcation.

(a) Random Designs. In Technometrics 1 (1959) the random designs technique is discussed in a number of papers (Satterthwaite (1959), Budne (1959), Youden, Kempthorne, Tukey, Box, Hunter, Satterthwaite, Budne (1959), Anscombe (1959)). The number of observations, n , is fixed beforehand, and for each observation the level of each independent variable is selected randomly to be 0 or 1, both with probability equal to .5. One may choose to select the levels of each variable independently between runs, or to select without replacement to achieve that each variable is at its high level in $n/2$ runs and at its low level in the remaining $n/2$ runs (and n should be even). In the literature no indication is given for the value of n . Various methods of analysis have been proposed, the most popular being to compute the "simple" estimates, i.e. take the difference between the averages of all observations when the variable under consideration is at its high level, and when it is at its low level, respectively.

We give only an extremely rough under-estimate of the number of runs needed to screen N variables in a random design experiment. Consider the number of different vectors of length n (n even) which contain $n/2$ entries equal to 1 and $n/2$ entries equal to 0. This number is $\binom{n}{n/2}$. Just to be able to construct a design without complete confounding between any of our N variables, which is what we need to be able to trace one variable, we already need at least n observations, with n such that $\binom{n}{n/2} \geq N$. We shall not go into the question, how many observations we need to be able to find k

non-zero variables; instead, we refer to Mauro and Burns (1984) who reject random balance designs in comparison to two stage group screening, which is our next subject.

(b) Two-Stage Group-Screening. The N variables are subdivided into G groups of size $g=N/G$ each (if N is not a multiple of G , the group sizes are taken as "evenly" as possible). As a first step, the G groups are studied by using a Plackett and Burman-(or PB-)design, see Kleijnen (1987, p. 302). The variables within each group are treated as a whole, i.e. they are varied simultaneously. The number of observations in the first stage is the smallest multiple of 4 that is greater than G , that is $G+4-(G \bmod 4)$. In the second stage the variables in the groups that in the first stage turn out to be important (if any), are submitted to a next PB-design. If s groups are left over after the first stage, then the number of observations in the second stage is $sg+4-(sg \bmod 4)$, assuming N is a multiple of G .

If k variables are important and these are all in different groups (worst case), then the total number of observations is approximately $G+kg=G+kN/G$. The optimal G is about $\sqrt{kN}$, resulting in $2\sqrt{kN}$ observations, as is easily verified. For small k and large N our procedure, which is of the order $k^2 \log N$, is superior.

Two-stage group-screening is described in detail by Mauro (1984) and Mauro and Burns (1984).

(c) Multi-Stage Group-Screening. Both Patel (1962) and Li (1962) generalize two-stage group-screening to its multi-stage analog. We shall briefly describe Patel's version; Li's approach differs only in detail.

In the first stage, 1 group of N variables is divided into g_1 groups of N/g_1 variables each, and analyzed in g_1+1 experiments (as in two-stage group-screening the variables within one group are varied simultaneously). Suppose the first stage turns out to give k_1 important groups. In the second stage, each of these groups is divided into g_2 groups of N/g_1g_2 variables and analyzed by using g_2 experiments. So, in the second stage a total number of k_1g_2 experiments are performed, resulting in (say) k_2 important groups. This is continued until we reach groups of size 1.

Patel neglects the difficulties arising from the fact that all divisions should result in integer numbers, so his results tend to be optimistic. He assumes that every variable has an a priori probability p of being important, and finds that in c stages approximately $1 + cNp^{1-1/c}$ experiments are needed. This comes down to an optimal c (straightforward differentiation) of $-\ln p$, and so an optimal number of experiments of $1 - Npe \ln p$. This number can be approximated by $ke \ln N$, while the number of observations in SB is approximately $k^2 \log N = k \ln N / \ln 2$. As $e > 1/\ln 2$, SB is superior.

(d) Jacoby and Harrison (1962)'s Sequential Bifurcation. In the original version of SB one starts by observing $y_{0|0}$, $y_{1|1}$ and $y_{2|1}$. A $\beta_{i|j}$ that is found to be positive, gives rise to observations $y_{2i-1|j+1}$ and $y_{2i|j+1}$, to find out whether $\beta_{2i-1|j+1}$ or $\beta_{2i|j+1}$ or both are positive. This is repeated until the stage of individual variables has been reached. The number of observations in the worst case can be computed analogously to the derivation of (3.1), and is equal to $2^{l+1} - 1 + 2k(m-l)$ if k out of 2^m parameters are positive, and $2^{l-1} < k \leq 2^l$ (for $k=0$, $l=1$). The number of observations is about twice as much as our modification of SB needs.

Example 5. Suppose we are dealing with 1024 variables, we have $m=10$. For $k=0,1,\dots,8$ the worst case number of runs is given in table 4, in which G2 stands for Two-stage group-screening, GM for Multi-stage group screening, JH for the Jacoby and Harrison (1962) Sequential Bifurcation, and SB for our version of Sequential Bifurcation.

k	0	1	2	3	4	5	6	7	8
G2	2	68	96	116	136	148	164	172	188
GM	2	19	34	48	61	73	84	95	106
JH	3	21	39	55	71	85	99	113	127
SB	2	12	21	29	37	44	51	58	64

Table 1. Maximum number of runs for given number of non-zero variables.

For G2, JH and SB we computed the number of runs in worst case, i.e. there is as few clustering as possible. For G2 we assumed that for the first stage we guessed the number of non-zero coefficients correctly. For GM we applied the formula $1-Np \ln p$ and rounded up to the next integer.

5. Discussion.

In this paper a modification of the Jacoby and Harrison (1962) Sequential Bifurcation is described, which is easy to perform and turns out to be very efficient. However, our model (2.1) is very restricted.

Two modifications can easily be performed: we may allow the regression parameters to be (slightly) negative; and we can restrict our search to great parameters. If we apply both modifications at the same time, we obtain the following model.

Assume that $\epsilon \geq 0$, $\delta \geq 0$, and the simulation outcome is given by

$$y = y(x_1, x_2, \dots, x_N) = \beta_0 + \beta_1 x_1 + \dots + \beta_N x_N \quad (5.1)$$

in which $\beta_l \geq -\epsilon$ ($l=1, \dots, N$), and we want to find those parameters β_l that are greater than δ . We can compute the (sums of) parameters $\beta_{i|j}$ in the same way as we did before. At any stage $\beta_{i|j}$ is the sum of 2^{m-j} parameters. If at least one of these parameters is greater than δ , and the other ones are all at least $-\epsilon$, then $\beta_{i|j} > \delta - (2^{m-j} - 1)\epsilon$. So adopting the rule to stop our search as soon as $\beta_{i|j} < \delta - (2^{m-j} - 1)\epsilon$, we may apply SB to the given situation as well.

A next modification would be to extend the method to observations with random error. A paper on this subject is in preparation.

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Figure 1. Example of error-free sequential bifurcation.

IN 1987 REEDS VERSCHENEN

- 242 Gerard van den Berg
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- 244 J.C. de Vos, W. Vervaat
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- 245 Arie Kapteyn, Peter Kooreman, Rob Willemse
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of subjective poverty definitions
- 246 J.P.C. Kleijnen, J. Kriens, M.C.H.M. Lafleur, J.H.F. Pardoel
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Criteria
- 247 D.B.J. Schouten
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Appendix: "Dynamic equilibrium in a competitive credit market: intertemporal contracting as insurance against rationing"
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